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EVALUATING THE SUITABILITY OF AUTOMOTIVE GAS OIL (DIESEL) FUEL FOR GAS TURBINE LP COMBUSTOR OPTIMUM PERFORMANCE ACROSS LEAN EQUIVALENCE RATIOS

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ABSTRACT - This work investigated the suitability of Automotive Gas Oil (AGO) fuel for optimum performance in the gas turbine engine lean premixed combustor at varying equivalence ratios. The process entails the numerical simulation of Automotive Gas Oil in a lean premixed combustor at different varying lean equivalence ratios. The computational fluid dynamics (CFD) technology using the ANSYS Fluent code (Academic Research CFD) version 16.2 was adopted to investigate the characteristic of the AGO during intense combustion activities at lean equivalence ratios (0.3,0.5,0.7 and 0.9) through the direct numerical simulation (DNS) processes. An AutoCAD pre-designed combustor was exported to the ANSYS Fluent GUI for fine tuning, gridding/mesh generation and discretisation process with the ANSYS Fluent solver while leveraging the finite difference method (FDM) to solve emerging complex equations. With the established combustor boundary conditions similar to an operational industrial gas turbine engine generating at 20MW. Simulations were conducted in both the steady-state and transient combustions regimes to evolve details of respective fuel combustion mannerism profiles on simulation convergence attainment. The obtained result detail of the dynamic, total pressures, acoustic amplitudes contours with CH* and OH* mass fractions for each fuel simulated under four equivalence ratios were analysed and tabulated. The outcome-based on parameters per equivalence ratio were analysed and compared to establish differences to proffer responses to the primary objectives of the research theme. The outcome revealed steady temperature range occurring between the equivalence ratio rate with the maximum temperature reading of 1044.38k at 252kPa at 0.5¢

KeyWords - ANSYS Fluent Code, AutoCAD, Automotive Gas Oil, Computational Fluid Dynamics, Direct Numerical Simulation Finite Difference Method, Steady State

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Introduction

The gas turbine is the engine of choice for propulsion and mostly mechanical drives in power generation, aviation, locomotive, the oil and gas as well as the maritime industries due to its ruggedness, its ability to operate under any environment and utilise multiple fuels as feedstock renders it an engine of choice amid its ready deployability. The continuous availability of the gas turbine engine is central to operational efficiencies of many industries who are overly dependent on it for propulsion and mechanical drives[18],[26]. Its non-availability, therefore, contributes significantly to overall operational cost overruns of most power generating plants, oil and gas, marine and aviation industries and this is due to frequent breakdown and the attendant cost of repairs or outright engine replacement. However, the stringent environmental regulations on gas turbines original equipment manufacturers (OEMs) on pollution control requirements precipitated the advent of the lean premixed combustion technology. The Control is geared toward the elimination of various kinds of oxides of Nitrogen (NO_x), Sulphides (SO_x), unburned hydrocarbons (UHC) and other pollutants from gas turbine effluents from the environment. It has been argued in the works of [10], [7] and [3] that, the gas turbines operating under the lean premixed technology are susceptible to the occurrence of a combustion phenomenon known as combustion instabilities.

The Combustion instabilities arise from the resonant interactions within the premixed combustors. The resonance leads to oscillations of the flowfield thereby inducing several undesirable effects: large-amplitude pressure and velocity oscillations resulting in thrust oscillations and structural vibrations increased heat fluxes at the combustor walls, flashback and flame blowoff [1], [6], [25], [7]. In the same vein,, [5],[3],[10],[13],[4],[14] stated that Combustion instability is the consequence of the positive coupling of the combustor excited acoustic field with the unsteady heat release of the flame during unstable combustion processes. They went a further step to emphasise that the unsteady heat release must be in phase with the acoustic- pressure- a condition necessary for energy addition to the unsteady motions

The resonant interactions are induced by a feedback loop between the oscillatory combustion process and one of the combustors natural acoustic modes. This phenomenon's inducing mechanics was qualitatively described by [21] as combustion instability occurs when the acoustic waves gain energy when the unsteady rate of heat input is in phase with pressure oscillations within the combustor.



Figure 1: Feedback Mechanism in a Combustion System. Source: Kulsheimer and Buchner (2002)

[1] argued that the performance of combustion system depend strongly on the physical and chemical properties of the fuels as this impacts on the combustion dynamics through flame type formation, heat release rate. The heat release eventually incenses the acoustic waves and consequently inducing the feedback mechanism that establishes the instabilities.

Several authors on gas turbine combustion have postulated the nexus between the composition of fuel types, combustion reactions and kinetics and equivalence ratios variation to combustion instabilities occurrences in gas turbine engines [10], [1], [19], [11].

In another instance, [23] argued on the futility of designing a combustor that would be stable during the entire operating range of the gas turbine or to predict the operating condition at which a given combustor would be unstable. This, according to the author, is due to the limited understanding of the fundamentals of combustion instability. [23] further stated that the development of the next generation lean premixed gas turbine (LPGT) Combustor would require design tools that would be based entirely on stability models to enable it to show the relationship between combustor design, operating ranges and combustion instability. Aside from the natural gas that is readily available in Nigeria, the automotive gas oil, also known as diesel fuel is readily and easily deployed as gas turbine feedstock as а substitute.[18],[[20],[22],[24] Argued on the susceptibility of certain fuels to combustion instabilities, a debilitating phenomenon plaguing the contemporary gas turbines with lean premixed combustion technology. The AGO or diesel fuel as an alternative feedstock to gas turbines requires that the combustion characteristics be established to enable the situation of an appropriate equivalence ratio(s) that typifies

its combustion mannerisms that would enable an appropriate design and appropriation of Wireless Sensory (WST) with Supervisory Control and Data Acquisition (SCADA) technology. This system would predict the onset of combustion instability that would instigate the adjustment of the feedstock charge (air and fuel) in appropriate ratios, thereby influencing the combustion characteristics and stem combustion instabilities and fuel consumption.

2 Materials and Methods

2.1 Materials

- ANSYS Fluent (Academic Research CFD) Version 16.2 leveraging finite difference methods(FDM) to solve the complex Navier-Stoke equation in viscid inviscid states as shown below;
- The simulation was carried out on an Intel (R) Core (TM) i-3-2377M CPU @ 1.7 GHz, 6BG memory RAM.
- Transient state is calculated until residues lower than 10⁻³ for all the variables except for the equation of energy (<10⁻⁶). A constant time step size (s) of 1 second and numbers of time step of 2500 with 20 max iterations/time step.
- CHEMKIN Collection, Release 3.6 providing gasphase diffusivities
- GRI-Mech 3.0 Gas-phase kinetic mechanism
- POLIMI Kinetic Mechanism for liquid formation.

2.2 Methods

The process entails the application of the following methodology which encapsulates the following procedures;

- Designing and applying dimensioning statistics of a typical gas turbine with AutoCAD software to develop the 2-D model with fundamental physics to capture useful results.
- Defining Boundary Conditions Two inlets (fuel, air), etc., Air mass flow rate, Inlet air temperature, Inlet total pressure of air, Inlet static pressure of air, the mass flow rate of fuel, Inlet fuel temperature, the velocity of fuel injection, Outlet Temperature, Pressure loss, Combustion efficiency, etc.
- Grid/Mesh Generation and discretization process by the ANSYS Fluent Solver
- Analysis Setup ANSYS Fluent (Academic Research CFD) version 16.2
- Turbulent Model adopted: Turbulent κ-ε model

The process entails the execution of series of convoluted DNS of AGO in stepwise process at different equivalence ratios that would lead to the determination of the following parameters is then analysed to draw inferences. This will entail the study of the following simulations outcome.

- i. Dynamic and Total Pressure magnitudes outlay of fuels at different equivalence ratios in the computational domain
- ii. Fuels Temperature Profiles at different equivalence ration across the computational domain
- Fuels Mass Fractions(OH*, C*, CH* display at various equivalence ratios within the LP Combustor domain at various equivalence ratios
- iv. Combustion Sound Pressures and Amplitudes of Fuels in different equivalence ratios across the domain.

The significant step in CFD analysis involves the definition of the computational domain(LP Combustor) for the CFD calculation as this allows the flow dynamics to be adequately developed to cover the entire length of the computational domain. The CFD is premised on the fluid flow governing equations-continuity, momentum and the energy equations.

2.3 Geometric model preparation:

The Computational Domain (LP combustor) was developed using the AutoCAD software with the following configuration(Figure 2) and exported to the ANSYS Fluent(Academic Research CFD) v.16.2 GUI for gridding and meshing. The model preparation was premised on a geometrical drawing of the combustors and mesh construction, and it played a significant role in the simulation accuracy and the solution convergence through its accuracy and stability of the numerical computation. Launching of the Meshing programme for the Grid/Mesh generation process through setting the relevance centre to Medium(RCM) under sizing and the midsize elements.



Figure 2: LP Combustor Dimensions

The mesh generation process presented the following details: A 2-D Axis symmetric mesh with 24,834 faces, 12,168 quadrilateral cells of mesh quality of 5.80670e-01 maximum orthogonal skew, and minimum orthogonal quality of 4.13782e-01 was adopted for the simulation (Figure 3, Tables 1 and 2) The mesh aspect ratio is 7.26027e+00. The nominal length of the combustor is 800mm, width 200mm, the air and fuel enters into the combustor separately and are premixed

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by the swirler which is positioned at an angle of 50 degrees to the air and fuel flow. The Swirler is made up of 8 vanes with the following configurations. The AutoCAD model of the combustor was exported into the simulation environment deploying the IGES format while the flow-field was created by ANSYS Design Modeller(ADM) with Boolean subtract function(Fig.3)



Figure 3: MeshedLayout of the LP Combustor

Table 1: LP Combustor Mesh	Generation Statistics
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Method	Triangles	Definitions
<u>Ci-i</u>	Size function =	
Sizing	proximity, relevance =	
	fine, smoothing = fine	
	minimum volume	
Volume statistics	(m3): 6.035354e-08,	Total volume (m3): 1.016065e-
(m3)	maximum volume	01
	(m3): 5.777815e-05	
	minimum face area	
T	(m2): 2.008038e-04	
Face area statistics	maximum face area	
(m2)	(m2): 9.971539e-03	
		Orthogonal Quality ranges from
	Minimum Ortnogonal	0 to 1, where values close to 0
	Quality = 4.13/82e-01	correspond to low quality.
	Manimum Ortha Cham	Ortho skew ranges from 0 to 1,
MIA P	F 90670a 01	where values close to 1
Mesh Quality	= 3.800/08-01	correspond to the low quality
Maximum Aspect	7 26027e+00	-
Ratio	7.200270100	
Cells	12168	
Faces	24834	
Nodes	12666	

Models Function Description of Governing Parameters adopted for the Investigation Solver Pressure based, absolute velocity formulation, transient time bases simulation

Table 2: Simulation Set-Up Details

	transient time bases simulation	
Model	 k – epsilon equation – standard model, Radiation – discrete ordinate, 	
Spark ignition	Initial radius – 0.0002, location – 0.169104, 0.0234036,	
Acoustic	Broadband noise sources	
scaled residuals	10-6 for all the equations	
	Transport model, Chemistry interaction – eddy	
	dissipation concept, volumetric reaction	
species	coupled with CHEMKIN option to allow for	
	significant species of combustion reactions	
	Kinetic reaction mechanism of the Gas	
W1	Research Institute (GRI) mechanism (Gas fuel)	
Kinetics reaction	and POLIMI Kinetic mechanisms (Liquid fuel)	
mecnanism.	both in Chemkin format	
Scheme	Couple	
	Gradient –Least square cell base	
	Pressure - Second Order Upwind	
Discretization	momentum – second order Upwind	
	others – first order upwind	
Solution control	Default	
Initialization	Standard	
Colculation	Time step size – 0.00001, numbers of time step	
Calculation	= 500, max iteration = 20	
Mach Scale	X-min(mm) -172, X- max(mm) 696	
iviesn scale	I I I I I I I I I I I I I I I I I I I	
	Y-min(mm) -2.8715e-31, Y-max(mm) 198.926	
Total Volume(m3)	Y-min(mm) -2.8715e-31, Y-max(mm) 198.926 1.016065e-01	
Total Volume(m3) Face Area Statistics	Y-min(mm) -2.8715e-31, Y-max(mm) 198.926 1.016065e-01 Minimum face area (m2): 5.090730e-04	

Table 3: Properties of Fuels Investigated and Initial Conditions Deployed

Fuel	Impeller diameter D (m)	Kinematics viscosity V @ 15 ⁰ C M ² /S	Rotation al speed N Rev/Sec	Rotational speed (N * 2π) Rad/Sec	Fuel inlet diameter (m)	Air inlet diameter (m)
AGO	0.008	2.5 x 10-6	1.25	7.853	0.015	0.10

D = 0.008, $D^2 = 0.000064$

The mass flow of air and that of the fuels were found using equations 1-5 respectively at an output power of 20000KW(20MW). This enables the details in Tables 4 for the fuel type

$$\dot{m}_{\text{fuel}} = \frac{P(KW)}{LHV_{\text{fuel}}} X 1000$$
 (1)

m'air =
$$\frac{\dot{m}_{fuel}}{MW_{fuel}} \phi / MW_{air} Xn_{stoich}$$
 (2)
 $\phi = \frac{FAR}{(FAR)_{stoic}}$ (3)

 $\label{eq:where FAR} \begin{array}{l} = \frac{\dot{m}_{fuel}}{\dot{m}_{air}} & (4) \\ \mbox{Stoichiometric is shown as follows;} \\ C_x H_{y+} A \left(O_2 + 3.76 N_2 \right) = x C O_2 + (\frac{y}{2}) H_2 O + 3.76 a N_2 \\ \mbox{where a} = x + \frac{y}{4} \mbox{ and } \end{array}$

$$(FAR)_{stoic} = \left(\frac{\dot{m}_{fuel}}{\dot{m}_{air}}\right)_{stoic} = \frac{1}{4.76a} \frac{(MW)_{fuel}}{(MW)_{air}}$$
 (5)

Where *P* is the Power output, LHV_{fuel} represent the Lower Heating Value of fuel, ϕ is the combustion equivalence ratio, n_{air} is the mole amount in stoichiometric-fuel-air combustion. The amount of simulations was limited to different premixed air-fuel ratios($\dot{m}_{air}/\dot{m}_{fuel}$) and *MW* is the molecular weight of fuel.

Table 4: Parameters for Automotive Gas Oil/ Diesel Mass Fuel-Air Flow Combustion at 20MW

		Diesel(AGO)					
	φ	M _{fuel}	M _{air}	Mair/Mfuel	FAR	Power Output	
Ī		kg/s	kg/s			KW	
ſ	0.3	0.457388	7.74631261	16.93597692	0.0590459	20,000	
	0.5	0.457388	4.64804892	10.16215756	0.0984043	20,000	
	0.7	0.457388	3.31934633	7.257178435	0.1377946	20,000	
	0.9	0.457388	2.581713251	5.644470889	0.177164524	20,000	

Table 5: Boundary Conditions

Гуре	Properties Diameter (mm) = 15mm, <u>Gas fuel</u> (Temperature 15°C (288K), pressure = 101325 P) <u>Liquid fuel</u> (Temperature 25°C (298K), pressure = 101325 P) P)			
Fuel inlet				
Air Inlet	Diameter (mmm) = 50mm, <u>Gas fuel</u> Temperature 15 ⁶ C (288K), pressure = 101325 P <u>Liquid fuel</u> (Temperature 25 ⁶ C (298K), pressure = 101325 P			
Dutlet	Diameter (m) = 0.06, Static pressure = 0			
Wall (Air)	Material = steel			
Wall (Fuel)	Material = steel			
Wall (Combustor)	Material = steel			
Wall (Outlet)	Material = steel			

Material = steel

Model κ-ε Turbulent

Wall (Swirler)

Motion/Fluid Type (Swirler Configuration) N = VRe/D2, Where N = Rotational speed in Rev/Sec, V =Kinematics viscosity (M2/S), Re = Reynolds number, D = impeller diameter. $V = \mu/\rho$ where μ = absolute or dynamic viscosity (NS/m2), ρ = density (Kg/m3) Re< 23000 – Laminar, 2300 < Re < 4000 - Transition, Re>4000 – Turbulence

2.4 Stepwise Procedure

The simulation was carried out using Computational fluid dynamics (CFD) software ANSYS Fluent 16.2 (academic version). Owing to the computational cost

and limited resources the geometry was modelled in 2-D space planar, ANSYS Fluent version 16.2 also has a limit to the maximum numbers of cells it can model. This poses a problem for further grid refinement.

Transient state is calculated until residues lower than 10^{-5} for all the variables except for the equation of energy (< 10^{-6}). A constant time step size (s) of $1e^{-05}$ second and numbers of time step of 200 with 20 max iterations/time step were adopted.





Figure 4: Magnifies Section of LP Combustor in discretization process

The Simulations were executed on two fronts taking cognisance of their respective physical dispositions. In allowing for large species of combustion reactions, transport model, chemistry interaction eddy dissipation concept and the volumetric reactions were all coupled with the CHEMKIN format. The CHEMKIN format contains the Kinetic reaction mechanisms of the Gas Research Institute (GRI), Gas Fuel Mechanism and the POLIMI kinetic mechanisms for liquid fuels

The spatial model adopted as stated earlier is 2-D Space. Due to the physical status of the fuel, the Solver was respectively set to pressure-based transient model and the pressure-based Steady model.

2.5 Solution Initialisation

This solver dependent (Steady State and Transient State). This is because the occurrence of flows is complex and non-linear. Several iteration processes were undertaken to observe simulation consistency and ultimately convergence. The convergence of a numerical process may be defined as the solution of the system of algebraic equations approaching the actual solution of the partial differential equation having the same initial and boundary conditions as the refined grid system. Retrieving Result of interest - (Distribution of flow rate, temperature, power and heat, pressure, etc.) and plot for respective parameters

Plots were retrieved per parameter per equivalence ratio for the fuel type analysed. Details were subsequently obtained from each plot and contours maps and translated in tabular formats.

3 Results and Discussion

The Automotive Gas Oil(Diesel) exhibited a consistent temperature profile range of (1042.49-1043.82) K across all equivalence ratios considered for the DNS at the combustor's reaction zone. Few works are reported in the literature on the impact of fuel types on combustion instabilities. Total temperature profile at 0.3ϕ exhibited that the incompressible liquid fuels displayed higher and steadier temperature profile through the combustor.

The LP combustion pressure at combustion chamber entry for the 0.3ϕ is 400kPa (4bars) declined to 300kPa. It was observed that simulations conducted for further equivalence ratios compared to 0.3ϕ shows decline in combustion dynamic pressure at 0.5¢ from 254.3kPa at 60cm downstream combustor length to 15kPa at 20cm at 0.9 ϕ (Table 6). The total temperature however, exhibited more stability within and across combustors on all Equivalence ratios. temperature difference within combustor is 0.88°K at 0.3 ϕ with a slight fluctuation difference of 0.78K at 0.5 ϕ to 0.63K at 0.9K at 0.9 ϕ across all Equivalence ratios simulated. Average Total temperature build of AGO across all equivalence ratios is 1042K. However, it was equally observed that the combustion total pressure peaked 766kPa at 0.3ϕ within 60cm downstream combustor (Tables 8). The pressure differential across equivalence ratios is highest at 0.3**b** upstream with a 360kPa fluctuating difference.

The work of [12] on methane combustion provides credence to this work.

[8], [1], [11], [16] stated that the highest temperatures during combustion are obtained upstream combustor (near nozzle), and hydrogen gas temperature was 2330K and the natural gas 2290k. On the other hand, [12] in their work obtained 1850K and had argued against the theoretical temperature of 1950k. The various temperature profiles as obtained by this study showed explicitly what was obtainable at various equivalence ratios and correlates with the work of [16] and [12].

[18] in their works observed that the dynamic and total pressures readings of incompressible liquid fuels- DPK and AGO, exhibits higher combustible dynamic pressures than the compressible gaseous fuels at a lower equivalence ratio at 0.3 φ with pressures reducing upstream combustor with a sudden spike in pressure at the most upstream. Another observation is decreasing pressures with increasing equivalence ratios.

The simulation findings ably aptly demonstrated the effect of equivalence ratio fluctuations on AGO during intense

combustion processes in gas turbine engines, while further providing a detailed characterisation of the fuel used for the study, as various combustion pressure and temperature details were obtained for each fuel (Tables 6,7and 8)

Table 6: Dynamic Pressure (Pa) Profile acrossEquivalence ratios for AGO fuel Combustion

Length within Combustor(m)	0.3φ	0.5φ	0.7φ	0.9 φ
0	400,000.00	127,659.60	63,000.00	35,714.00
0.2	300,000.00	100,000.00	49,000.00	26,857.00
0.4	195,833.00	56,383.00	26,000.00	15,147.00
0.6	773,529.00	254,383.00	124,500.00	70,000.00

Table 7: Total Temperature(K) Profile across Equivalence ratios for AGO Combustion

Length within Combustor(m)	0.3φ	0.5φ	0.7φ	0.9 φ
0	1,043.82	1,043.60	1,043.22	1,042.06
0.2	1,044.41	1,044.10	1,043.68	1,042.69
0.4	1,044.41	1,044.21	1,043.84	1,042.69
0.6	1,044.70	1,044.38	1,043.84	1,042.69

Table 8: Total Pressure(Pa) Profile across Equivalence Ratios AGO Gas Combustion

Length within Combustor(m)	0.3φ	0.5φ	0.7φ	0.9φ
0	306,666.70	100,000.00	50,000.00	31,023.60
0.2	459,999.00	150,000.00	72,916.70	42,362.20
0.4	333,333.00	112,500.00	54,166.67	35,748.03
0.6	766,666.00	252,083.30	122,916.70	73,385.80

4 Conclusion

This work detailed the maximum temperature and pressures obtainable from AGO and at what instance of equivalence ratios, they were obtained. [15] in their work stated that the gas turbine exhaust temperatures hoover around 2073.15K-2273.15K, which they considered too hot for the nozzle guide vanes of the turbine.[2]argued That in reference to the

Zeldovich equations for thermal NO_x , that the NO_x is generated to the limit of available oxygen at about 200,000ppm at temperatures above 1573.5K and that no NO_x is produced at a temperature below 1033.15K. With this information, the gas turbine primarily fueled by AGO could have its an AGO Combustor specific with wireless sensory system (WSR) and SCADA that would enable the monitoring and control of combustion instabilities signals as combustion temperature approach disturbing level through appropriate adjustments in the speed, volume and quantity of air and fuel for combustion.

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